

Universal Behavior Of Lyapunov Exponents In Unstable Systems

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Abstract

We calculate the Lyapunov exponents in a classical molecular dynamics framework. The system is composed of few hundreds particles interacting either through Yukawa (Nuclear) or Slater-Kirkwood (Atomic) forces. The forces are chosen to give an Equation of State that resembles the nuclear and the atomic ${}^4\text{He}$ Equation Of State respectively near the critical point for liquid-gas phase transition. We find the largest fluctuations for an initial "critical temperature". The largest Lyapunov exponents λ are always positive and can be very well fitted near this "critical temperature" with a functional form $\lambda \propto |T - T_c|^{-\omega}$, where the exponent $\omega = 0.15$ is independent of the system and mass number. At smaller temperatures we find that $\lambda \propto T^{0.4498}$, a universal behavior characteristic of an order to chaos transition.

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The phenomena of phase transitions have been always a subject of great interest for many (generations of) physicists. Very recently there has been a large interest in studying what happens when the system is not composed of 10^{23} particles and confined in a box but, on the opposite, is composed of few hundred particles that are not confined. This interest has born first in heavy ion collisions where one would like to study the Nuclear Equation of State (NEOS) [1]. In the nuclear case it is not possible to study the infinite number of particles case (apart in stars with the obvious difficulties), so one feasible way is to perform proton-nucleus or nucleus-nucleus collisions. In this manner it is possible to heat up and to explore different densities of the nuclei. Of course the problem is complicated apart from the fact of having a small number of particles, also from the presence of Coulomb force, angular momentum and from the approximate knowledge of the "thermodynamical parameters", i.e. temperature, density and pressure [2–4]. Similar problematic can be found in the study of metallic clusters and/or fullerenes [5]. One of the first questions that arises is: does it make sense to speak about phase transitions for a system made of 100-400 particles? To answer this question the authors of refs. [3,5] and [6] have solved the exact classical many body problem (Classical Molecular Dynamics-CMD) numerically for particles interacting through two body forces. In particular preparing 100 particles in the ground state and giving to the particles an excitation energy (or temperature T) the following results are found:

1) for a given initial temperature T_c the system undergoes multifragmentation [3,6,7]. The resulting mass distributions display a power law $Y(A) \propto A^{-\tau}$ with $\tau = 2.23$, which is exactly the value predicted in the Fisher droplet model for a system near the liquid-gas phase transition point [8]. Other critical exponents have also been estimated within the same model [7]: $\gamma = 0.86$, $\beta = 0.33$ [9]. Similar estimates but for experimental data on Au+C collisions at 1 GeV/nucleon [4] give also reasonable values of all the exponents;

2) at the same temperature, fluctuations in the mass distribution are maximum. This is revealed through the study on an event by event analysis of intermittency signal, factorial moments and Campi's plots [6,10,11];

3) the "critical temperature" follows the scaling law $T_c/|E_b| = \text{constant}$ [5]. Where E_b

is the binding energy of the system (10.5 MeV for nuclei, 9.5 eV for C60 fullerenes and 50.5 0K for 4He molecules);

4) at very small temperatures or, equivalently, small excitation energies, the events are typical evaporation like events, i.e. with a final mass distribution composed of a big fragment and many small ones : monomers, dimers etc.

For some initial conditions the system displays large fluctuations, thus we expect that other indicators of fluctuations -the Lyapunov exponents - should be positive. The values of the Lyapunov exponents for systems undergoing a phase transition are not known (yet). In particular the relationship between thermodynamical and dynamical properties have not been exhaustively explored. Ours is the first estimate of the Lyapunov exponents for systems exhibiting a critical behavior (possibly because of a liquid-gas phase transition). In a previous exploratory work, but for a two dimensional system and in the mean-field approximation, the largest Lyapunov exponents were calculated in the spinodal region [12]. It is well known, however, that the mean-field approximation gives a rough estimate of the critical exponents [8], thus it is interesting to estimate their values in CMD.

We can summarize the main results of this work as follows:
independently of the studied system, i.e. nuclei, helium molecules, the largest Lyapunov exponents satisfy, similarly to the Landau theory of phase transitions, the relation

$$\lambda \propto |T - T_c|^{-\omega}, \quad T \sim T_c \quad (1)$$

where $\omega = 0.15 \pm 0.04$.

At smaller temperature the Lyapunov exponents scale as

$$\lambda \propto T^{\frac{\ln 2}{\ln \delta}}, \quad (2)$$

with $\delta = 4.669...$ the Feigenbaum constant [13] which indicates a typical transition from order to chaos [14,15].

Our studies are based on direct numerical simulation of an expanding system in classical molecular dynamics. In particular we have studied a "nuclear" system where "neutrons"

and "protons" interact through Yukawa potentials. Details of the forces can be found in refs. [3,16]. The parameters entering the potentials have been fitted in such a way to have a ground state density of 0.16 fm^{-3} , a binding energy of -16 MeV/nucleon for an infinite system. For finite systems the binding energy is -10.5 MeV/nucleon without Coulomb. In this work we will discuss the parameter set that gives a soft EOS, i.e. compressibility $K=200$ MeV [16] and the Coulomb interaction will be neglected. We notice that the use of the set corresponding to a stiff EOS, $K=380$ MeV, gives the same results.

We have also studied He atoms interacting through the potential [17]

$$v(r) = 5.67 \cdot 10^6 e^{-21.5(r/\sigma)} - 1.08 \left(\frac{\sigma}{r}\right)^6, \quad (3)$$

where $\sigma = 4.64$ Angstrom and $v(r)$ is in Kelvins.

In order to calculate the largest Lyapunov exponents [15] we first define the following metric in phase-space

$$d(t) = \sqrt{\sum_{i=1}^N [\alpha (\mathbf{r}'_1(t) - \mathbf{r}'_2(t))^2 + \beta (\mathbf{p}'_1(t) - \mathbf{p}'_2(t))^2]_i}, \quad (4)$$

where the sum runs over all the N particles of the system, the subscript 1 and 2 refers to two events that at time $t=0$ differ of an infinitesimal quantity $d(0) = 10^{-6}$ or less. The \mathbf{r}' and \mathbf{p}' are scaled positions and momenta. In our case

$$\mathbf{r}'(t) = \mathbf{r}(t)/R_{rms}, \quad (5)$$

$$\mathbf{p}'(t) = \mathbf{p}(t)/P, \quad (6)$$

where R_{rms} is the root mean square radius and $P = \sqrt{2mT}$ is an average momentum, being m the nucleon (or the atom) mass and T the initial temperature (see below). Normally the Lyapunov exponents are calculated for systems bound in phase-space. This is not always the case in our simulations since for high excitation energy the phase-space explodes. In order to be certain of the soundness of our results we calculated the metric for three cases: 1) $\alpha=1$ and $\beta=1$; 2) $\alpha=1$ and $\beta=0$; 3) $\alpha=0$ and $\beta=1$. The results are independent on the choice of the metric, cases 1-3, as it should be.

The Lyapunov exponents λ are obtained from the relation

$$d(t) = d(0) e^{\lambda t} . \quad (7)$$

In our numerical simulations we prepared a system of 100 particles in their ground state. Then we distributed the momenta of the particles according to a Maxwell-Boltzmann distribution at temperature T and let the system evolve in time by solving the classical equations of motion. At each temperature 100 events were generated. For each event (test event) ten other events were generated, each event differing from the test event of $d(0)$. The exponents were obtained by averaging over all the events. In order to get λ numerically, we calculated the ratio $d(t)/d(0)$ and fitted its exponential growth. As a check we estimated also

$$\dot{d}(t)/d(t) = \lambda . \quad (8)$$

In figure 1 we plot typical evolutions of $d(t)/d(0)$ at three temperatures $T=2, 5$ and 20 MeV for the nuclear system. We see that the distance increases exponentially with time and can be very well fitted with a straight line (in a semilog plot) whose slope is just the Lyapunov exponent. The same results are found by using eq.(8). In general we get Lyapunov exponents which are always positive at all temperatures and have a maximum value at $T \sim 4.5$ MeV. A similar behavior is found for the atomic case with a maximum at $T \sim 21.8$ 0K . In order to compare such different systems like nuclei or atomic He, we scale temperatures and times with typical values of the different systems. Usually one scales with the values obtained at the critical point. Since we do not know these values a priori, we scale the temperature with the absolute value of the binding energy and the (inverse) times with a typical value λ_0

$$\lambda_0 = \sqrt{2|E_b|/m/R_0} . \quad (9)$$

Recall that in order to derive the EOS [8] one needs to know the hard core radius and the depth of the two body potential. These quantities are proportional to the average equilibrium distance between particles $R_0 = R/A^{\frac{1}{3}}$, - where R is the radius of the system and A the mass number - and to the binding energy. In our case $\lambda_0 = 0.155$ c/fm for

the nuclear case and $\lambda_0 = 8.82 \cdot 10^{-5} \alpha c/a_0$ for the atomic one, being α the fine structure constant, c the speed of light and a_0 the Bohr radius. In figure 2 we plot the Lyapunov exponents at each initial temperature (in units of their typical values) for the nuclear (circle symbols) and atomic cases (squares). Note that the maximum value of λ is obtained at the initial scaled temperature

$$T_c/|E_b| \sim 0.43 \quad (10)$$

for both systems. For such temperatures the systems undergo multifragmentation and a power law in the mass distribution and factorial moments is found [3,6]. Thus our result confirms that in this temperature region fluctuations are largest. Inspired by the Landau theory of phase transition, we parametrized the exponents according to eq.(1). The fit is also displayed in figure 2 (full and dashed curves). The same value $\omega = 0.15 \pm 0.04$ was used in both cases. Note the good agreement with the scaled λ at all temperatures but the lowest ones. For such small temperatures there is not any multifragmentation of the system, indeed the mass distribution reveals a typical cases of evaporation. Using the same language as in the theory of phase transitions we could say that the small temperature cases explore densities and pressures outside the spinodal region. Note that the absolute values of the scaled exponents differ of less then 30% for the two cases. Correspondingly the two fits differs only for a multiplicative constant C . The reason for such a small discrepancy is due to the fact that in the nuclear case we have two fluids, neutrons and protons. We will discuss this point in more detail in a following publication [18]. We also stress that these results are independent on the chosen metric, i.e. in the values of α and β in eq.(4). We have also tested the results by changing the mass of the fragmenting system. The Lyapunov exponents remained the same for masses ranging from 50 to 400 particles [18]. The uncertainties reported in figure 2 are of the order of $\sim 10\%$.

A scaling law of Lyapunov exponents of the kind

$$\lambda \propto (A - A^*)^{\ln 2 / \ln \delta} = (A - A^*)^{0.4498}, \quad (11)$$

where A is a control parameter and $\delta = 4.669\dots$ the Feigenbaum constant [13], is typical of order to chaos transitions. The value A^* is the critical value which indicates the onset of chaos. The expression (11) was initially found in the logistic map [14], but various experiments have confirmed its general validity [15]. In our case the largest Lyapunov exponents λ are positive for all finite temperatures, i.e. the dynamics is always chaotic, but they tend to zero as the temperature T goes to zero. Actually for $T=0$ the systems are frozen in their ground state and λ vanishes. Thus chaos starts at $T > 0$.

In figure 3 we plot a magnification of figure 2 for very small temperatures. The full curve is the expression (11) multiplied by a constant fitted on the numerical points. In this case the control parameter is the scaled temperature and A^* corresponds to $T=0$. The agreement is really impressing for both systems up to $T/|E_b| \sim 0.1$.

We can try to understand this behavior by recasting our microscopic dynamics in terms of a phenomenological macroscopic model. At very low temperatures one gets essentially evaporation events. Considering a discrete map, at time n the system evaporates z_n particles and it will continue evaporating qz_n particles until the excitation energy is zero. The number of evaporated particles at time $n+1$ is thus $z_{n+1} = (1 + q)z_n$. If z_0 is the final number of particles and we assume that the number of evaporated particles decreases linearly with time because the excitation energy is decreasing, we obtain $z_{n+1} = (1 + q)z_n(1 - z_n/z_0)$. This is nothing else than the logistic map if $1 + q = A$ and $x_n = z_n/z_0$.

Thus we have two different mechanisms at play. The first one for small temperatures gives a transition from order (the ground state) to chaos and has a dynamical origin. The second mechanism, for reduced temperatures larger than 0.1 has a thermodynamical origin appropriate for a second order phase transition. Loosely speaking we have given evidence for "critical chaos" in the latter case.

In conclusion, in this work we have calculated the largest Lyapunov exponents as a function of the initial temperature for an expanding system composed by 100 particles in the framework of classical molecular dynamics. We have shown that these exponents are always positive and have their largest value at a temperature of $\sim 4.5 \text{ MeV}$ for the nuclear

case and $\sim 21.8 \text{ }^0K$ for the atomic one. We have also demonstrated that the λ obey to universal scaling laws. They fulfill the relation $|T - T_c|^{-\omega}$, $\omega = 0.15 \pm 0.04$, similarly to the Landau theory of phase transitions near the critical point. At the same time for smaller temperatures (evaporation events) Lyapunov exponents exhibit a general transition from order ($T = 0$) to chaos ($T > 0$). We feel that further investigations following the ideas presented in this paper may help our understanding of order and disorder in classical systems and, after all, in (part of) Nature itself.

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FIGURES

FIG. 1. The ratio $d(t)/d(0)$ is plotted as a function of time at three initial temperatures $T = 2, 5, 20 \text{ MeV}$ for the nuclear system. The dashed lines are fits whose slope give the typical λ for these temperatures after averaging over hundreds of events.

FIG. 2. The scaled largest Lyapunov exponents λ/λ_0 are plotted vs. the scaled initial temperature $T/|E_b|$ for the nuclear (circles) and the atomic (squares) case. The full and dashed lines are fits obtained with the functional form $C|T - T_c|^{-\omega}$ where $\omega = 0.15 \pm 0.04$. The parameters of the fits are $C=0.25$ and $C=0.3$ for the nuclear and atomic case respectively. See text for further details.

FIG. 3. A magnification of figure 2 at very small temperatures. The full curve is a fit with the functional form $K T^{0.4498}$ where $K = 0.55$ is the fitted parameter. See text for further details.